PHILOSOPHICAL MAGAZINE B, 1996, VOL. 73, NO. 6, 931–933

SUBJECT INDEX

Vol. 73

	PAGE
a-$Si_{1-x}C_x$: H films	429
a-Si : H, $1/f$ noise	707
a-Si : H from helium silane	261
a-SiN_x : H films	487
a-SiN_x : H, p–i–n structure	543
a-SiO_x : H photoluminescence	799
Absorption-edge shift	213
AgGa liquid	231
Alkali–metalloid alloys	585
Aluminium alloys with films	445
Amorphous carbon doped with copper	715
Anisotropic potentials	95
Anodizing multilayer alloys	297
$ASnO_3$	33
Binary alloys, transition temperature	737
Buckingham-type potential	41
Carbon spheres, nano-sized	905
$Ce_3Bi_4Pt_3$, properties model	525
Charge transfer in binary alloys	737
Charge trapping, organic photoconductor	779
Chemical impurity-dislocations	845
Cluster interactions	107
Coarsening simulations	409
Cohesive properties	893
Conductance fluctuations in a–Si : H	707
Covalent materials	85
Critical exponents in superconductors	619
Crystallization of amorphous films	289
Cyclotron resonance deposition	487
Databases for potentials	191
Defect creation and annealing in a-Si : H	261
Defect–dopant interaction	245
Disordered polymeric materials	153
Disordered system transport	201
Distributed multipole	117, 127
Dopants in hydrogen-free a-Si	245
Double-well potentials	657
Electrical conductivity fluctuations	619
Electrical resistivity of liquid metal	231
Electron localization	325
Empirical potentials	1
Fermions, two-dimensional Monte Carlo	555
Fitting and testing potentials	191
Force field parameters, large Q	153

Germanium, amorphous by irradiation 677
$GeSe_2$, amorphous 213
$Ge_{20}Te_{80-x}Bi_x$ amorphous films 383
Grain growth simulation 395, 409
Graphite, iron on surface 611

Hägg's rule, cubic phases 833
Heisenberg spin-1 chains 601
Hexa-aluminates 21
High-temperature superconductivity 223, 793
Hopping transport 201, 873
Hydrogen diffusion 503
Hydroxide ions 49

Interatomic potentials, issue 1–199
Inversion layers, SiC 325
Ion implantation in organic films 367
Ion irradiation for amorphization 677
Ionic conduction in glasses by AgS 349
Ionic materials 1
Iron as a surface impurity 611

Jahn–Teller 85

Kondo insulator 525

$LaFe_xNi_{1-x}O_3$ conduction 873
Laguerre model 395, 409
LiH molecule 175
Local-harmonic method for properties 627
Localized spins, thermostatics 745
Localized states at dislocations 845
Lone pair 95

Metal ions in anodic films 445
$MgSiO_3$ 41
Mo, liquid 309
Molecular solids 127
Molecular ionic materials 147
Monte Carlo phase transition 59
Muon spin relaxation in solid oxygen 689

Nanocrystalline materials 861
NiTi, martensitic and electronic structure 511

OH polarizability 49
Optical absorption, carbon 715
Optical and electrical properties 277
Optical properties of a-SiN films 339
Oxide-catalytic carbonization 905
Oxygen doping 223
Oxygen, magnetic structure 689

Paramagnet, ideal 745
Pd_3Fe, nanocrystalline 503
PdTi, martensitic and electronic structure 511
Peak effect in superconductors 793
Peptide conformation 139

Perchlorates and phosphates 147
Perovskites, domain-wall model 657
Photoluminescence, a-Si 799
Plasma-enhanced CVD, SiN 817
Plasmons and valence band 763
p–n transition absence 383
Polar molecules 117
Polarization effects 139
Poly (*N*-vinylcarbazole) 779
Poly (*p*-phenylene vinylene) 367
Polymethylmethacrylate, ion irradiation 763

Quasicrystals, tiling 641

Resistivity, alloys 585

Sb–Sn–O amorphous films 277, 289
Si–B parameters 71
Silver phosphate glasses 349
SiN, amorphous films 339
SiN, electrical conduction 723
Solute diffusion, fast 833
Spinel potentials 21
Stannate potentials 33
Statistical mechanics for materials 627
Superheated liquid metal 309
Surface energies and structures 163
Surface steps as interacting fermions 555
Surface waves in films 669

Tight binding 71
Tiling, random structure 641
Transient photoconductivity 429, 543
Tunnelling currents, SiN 723
Two- and three-body potentials 163

UO_2 cohesion 893

Valence band approach 175
Valve metals 297
Vanadium Warwickites 601
Vortex lattice melting 793
VO_2 59

Water potentials 107

X-ray simulation, nanocrystalline 861

YIG films 669

PHILOSOPHICAL MAGAZINE B, 1996, VOL. 73, No. 6, 935–940

INDEX OF AUTHORS (WITH TITLES)

Vol. 73

PAGE

Adriaenssens, G. J., *see* Yan, B.
Aida, M. S., Attaf, A., and Benkhedir, M. L.: The optical properties of sputtered amorphous silicon nitride films: effect of RF power 339
Alexandrov, I. V., and Valiev, R. Z.: Computer simulation of X-ray diffraction patterns of nanocrystalline materials 861
Allan, N. L., *see* Hines, R. I.
Andre, B., *see* Marc, N.
Anokhin, A. O., Galperin, M. L., Gornostyrev, Y. N., Katsnelson, M. I., and Trefilov, A. V.: The effect of electronic localized states at dislocations on the 'chemical' impurity–dislocation interaction 845
Attaf, A., *see* Aida, M. S.

Baram, P. S., and Parker, S. C.: Atomistic simulation of hydroxide ions in inorganic solids 49
Bayley, P. A., and Marshall, J. M.: Transient photoconductivity in a-$Si_{1-x}C_x$:H thin films 429
Benkhedir, M. L., *see* Aida, M. S.
Bermejo, F. J., Cox, S. F. J., Mompeán, F. J., García-Hernández, M., Senent, M. L., and Martínez, J. L.: Muon spin relaxation in condensed oxygen 689
Bhatia, K. L., Singh, M., Kishore, N., and Suzuki, M.: Electronic conduction in Bi-modified amorphous thin films of $Ge_{20}Te_{80-x}Bi_x$ exhibiting an absence of a p–n transition 383
Bigot, B., *see* Petit, T.
Bihlmayer, G., Eibler, R., and Neckel, A.: Martensitic phase transformation and electronic structure of NiTi and PdTi 511
Birtcher, R. C.: Energy-dependent amorphization of Ge by Ne, Ar or Kr ion irradiation 677
Bishop, A. R., *see* Bussmann-Holder, A.
Blackstead, H. A., and Dow, J. D.: Evidence of the direct role of dopant oxygen in high-temperature superconductivity 223
Blank, H.: Hägg's rule and fast solute diffusion in cubic transition-metal phases . 833
Boechat, B., *see* Continentino, M. A.
Borges, H. A., *see* Continentino, M. A.
Botchkerav, A. E., *see* Mohammad, S. N.
Botchkerav, A. E., *see* Tao, M.
Bourbie, D.: Theory of hopping transport in disordered systems 201
Bredas, J. L., *see* Moliton, J. P.
Bussmann-Holder, A., and Bishop, A. R.: Time-dependent evolution of double-well potentials to model structural anomalies 657

Clancy, P., *see* Rasband, P. B.
Continentino, M. A., Fernandes, J. C., Guimaraes, R. B., Boechat, B., Borges, H. A., Valarelli, J. V., Haanappel, E., Lacerda, A., and Silva, P. R. J.: Strongly disordered Heisenberg spin-1 chains: vanadium warwickites 601
Coombes, D. S.: Deriving intermolecular potentials for predicting the crystal structures of polar molecules 117
Cooper, B. R., *see* Peng, S. S.

0141–8637/96 $12·00 © 1996 Taylor & Francis Ltd.

Cooper, D. L., and Thorsteinsson, T.: A modern valence bond approach for interatomic potentials 175
Cormack, A. N., *see* Park, J. G.
Cox, S. F. J., *see* Bermejo, F. J.
Cutroni, M., Mandanici, A., Piccolo, A., Fanggao, C., Saunders, G. A., and Mustarelli, P.: Ionic conduction in silver phosphate glasses doped with silver sulphide 349

Dent, A. J., *see* Müller, G.
Derst, G., *see* Müller, G.
Dimova-Malinovska, D., *see* Zacharias, M.
Dobson, B. R., *see* Müller, G.
Dow, J. D., *see* Blackstead, H. A.
Drew, M. G. B., *see* Slater, B.

Eibler, R., *see* Bihlmayer, G.
Eliat, A., *see* Yan, B.
Elser, V.: Random tiling structure of icosahedral quasicrystals 641

Fanggao, C., *see* Cutroni, M.
Fernandes, J. C., *see* Continentino, M. A.
Fernandez, M., *see* Garcia, S.
Flavell, W. R., *see* Hines, R. I.
Friend, R. H., *see* Hamer, P. J.

Gale, J. D.: Empirical potential derivation for ionic materials 3
Galperin, M. L., *see* Anokhin, A. O.
Garcia, S., Martin, J. M., Fernandez, M., Martil, I., and Gonzalez-Diaz, G.: Properties of a-SiN_x:H films deposited at room temperature by the electron cyclotron resonance plasma method 487
García-Hernández, M., *see* Bermejo, F. J.
Gasser, J. G., *see* Vinckel, J.
Gatto, M., *see* Kojima, M.
Geertsma, W.: On the resistivity of alkali–metalloid alloys 585
Gonzalez-Diaz, G., *see* Garcia, S.
Gornostyrev, Y. N., *see* Anokhin, A. O.
Greaves, G. N., *see* Müller, G.
Guimaraes, R. B., *see* Continentino, M. A.

Haanappel, E., *see* Continentino, M. A.
Habazaki, H., Shimizu, K., Skeldon, P., Thompson, G. E., and Wood, G. C.: The incorporation of metal ions into anodic films on aluminium alloys . . . 445
Habazaki, H., Skeldon, P., Thompson, G. E., Wood, G. C., and Shimizu, K.: Anodizing of multilayer alloy films formed by sputter-deposition of valve metals 297
Hamer, P. J., Pichler, K., Harrison, M. G., Friend, R. H., Ratier, B., Moliton, A., Moratti, S. C., and Holmes, A. B.: Optical studies of chemical doping achieved by ion implantation in poly (*p*-phenylene vinylene) 367
Hao, Y. G., *see* Peng, S. S.
Harrison, M. G., *see* Hamer, P. J.
Heine, V., *see* Payne, M. C.
Hellmich, W., *see* Müller, G.
Hines, R. I., Allan, N. L., and Flavell, W. R.: Potentials for B-metal compounds: the stannates $ASnO_3$ (A = Ca, Sr or Ba) and SnO_2 33
Hirscher, M., *see* Mössinger, J.
Holmes, A. B., *see* Hamer, P. J.
Horsfield, A.: Bond order potentials for the atomistic simulation of covalent systems 85
Horsfield, A. P., *see* Rasband, P. B.

Hucho, C., and Levy, M.: On the peak effect and vortex lattice melting in $YBa_2Cu_3O_{7-\delta}$ 793
Hugel, J., *see* Vinckel, J.

Iguchi, E., *see* Jung, W. H.
Ivanov-Omskii, V. I., Tolmatchev, A. V., and Yastrebov, S. G.: Optical absorption of amorphous carbon doped with copper 715

Jackson, R. A., *see* Telfer, G. B.
Johanson, R. E., Scansen, D., and Kasap, S. O.: $1/f$ conductance noise in n-type amorphous silicon 707
Jug, G.: Surface steps as interacting fermions: an approach to the disordering of surfaces with sublattices 555
Jung, W. H., and Iguchi, E.: Transition from hopping conduction to band conduction in $LaFe_xNi_{1-x}O_3$ 873
Jussiaux, C., *see* Moliton, J. P.

Kalbitzer, S., *see* Müller, G.
Kang, Z. C., and Wang, Z. L.: Mixed-valent oxide-catalytic carbonization for synthesis of monodispersed nano sized carbon spheres 905
Kasap, S. O., *see* Johanson, R. E.
Kato, H., *see* Kojima, M.
Katsnelson, M. I., *see* Anokhin, A. O.
Khalil, A. E.: Critical exponents of conductivity fluctuations in high-temperature superconductors 619
Kihn, Y., *see* Moliton, J. P.
Kishore, N., *see* Bhatia, K. L.
Kobayashi, K., *see* Shimizu, K.
Kojima, M., Kato, H., and Gatto, M.: Optical and electrical properties of amorphous Sb–Sn–O thin films 277
Kojima, M., Kato, H., and Gatto, M.: Crystallization of amorphous Sb–Sn–O thin films 289
Kronmüller, H., *see* Mössinger, J.
Krötz, G., *see* Müller, G.

Lacerda, A., *see* Continentino, M. A.
Lazzaroni, R., *see* Moliton, J. P.
Lemaignan, C., *see* Petit, T.
LeSar, R., and Rickman, J. M.: Finite-temperature properties of materials from analytical statistical mechanics 627
Lever, R., *see* Marc, N.
Levy, M., *see* Hucho, C.
Lhost, O., *see* Moliton, J. P.
Li, D., *see* Tao, M.
Li, D., *see* Mohammad, S. N.
Liebling, T. M., *see* Telley, H.
Lugomer, S., Maksimović, A., and Stipancić, M.: Laser-induced bursts of subsurface superheated liquid Mo 309

Mac Dónaill, D. A., and Morton-Blake, D. A.: Polarization effects on amino-acid and peptide conformations 139
Maksimović, A., *see* Lugomer, S.
Mandanici, A., *see* Cutroni, M.
Marc, N., Moisan, J-Y., Andre, B., and Lever, R.: Charge trapping in an organic photoconductor: poly (*N*-vinylcarbazole) doped with 2,4,7-trinitrofluorenone. 779
Marshall, J. M., *see* Bayley, P. A.
Martil, I., *see* Garcia, S.
Martin, J. M., *see* Garcia, S.

Martínez, J. L., *see* Bermejo, F. J.
Meaudre, M., *see* Vignoli, S.
Meaudre, R., *see* Vignoli, S.
Meenan, P., *see* Telfer, G. B.
Mitchell, G. R., *see* Rosi-Schwartz, B.
Mocellin, A., *see* Telley, H.
Mohammad, S. N., Tao, M., Park, D. G., Botchkarev, A. E., Li, D., and Morkoç, H.: Composition and conduction properties of silicon nitrides deposited by plasma-enhanced ultra-high-vacuum chemical vapour deposition 817
Mohammad, S. N., *see* Tao, M.
Moisan, J-Y., *see* Marc, N.
Molitan, A., *see* Hamer, P. J.
Moliton, J. P., Jussiaux, C., Trigaud, T., Lazzaroni, R., Lhost, O., Bredas, J. L., Kihn, Y., and Sevely, J.: Relation between plasmons and the valence-band density of states in polymethylmethacrylate: influence of ion irradiation on damage selectivity 763
Mompeán, F. J., *see* Bermejo, F. J.
Moratti, S. C., *see* Hamer, P. J.
Morel, B., *see* Petit, T.
Morkoç, H., *see* Mohammad, S. N.
Morkoç, H., *see* Tao, M.
Morton-Blake, D. A., *see* Mac Dónaill, D. A.
Mössinger, J., Hirscher, M., and Kronmüller, H.: Diffusion of hydrogen in nanocrystalline Pd_3Fe 503
Müller, G., Hellmich, W., Krötz, G., Kalbitzer, S., Greaves, G. N., Derst, G., Dent, A. J., and Dobson, B. R.: Dopant–defect interactions in hydrogen-free amorphous silicon 245
Murrell, J. N.: Towards a general strategy for global interatomic potentials for elemental solids, surfaces and clusters 163
Mustarelli, P., *see* Cutroni, M.

Nagels, P., *see* Tichý, L.
Neckel, A., *see* Bihlmayer, G.
Nobre, F. D., and Tsallis, C.: Localized-spins ideal paramagnet within non-extensive thermostatistics 745

Ouisse, T.: Electron localization and noise in silicon carbide inversion layers . . 325

Park, D., *see* Tao, M.
Park, D. G., *see* Mohammad, S. N.
Park, J. G., and Cormack, A. N.: Potential models for multicomponent oxides: hexaaluminates 21
Parker, S. C., *see* Baram, P. S.
Pasturel, A., *see* Petit, T.
Payne, M. C., Robertson, I. J., Thomson, D., and Heine, V.: *Ab initio* databases for fitting and testing interatomic potentials 191
Peng, S. S., Cooper, B. R., and Hao, Y. G.: Modelling of adsorption of iron impurities at the surface of graphite 611
Petit, T., Morel, B., Lemaignan, C., Pasturel, A., and Bigot, B.: Cohesive properties of UO_2 893
Piccolo, A., *see* Cutroni, M.
Pichler, K., *see* Hamer, P. J.
Price, G. D., *see* Stuart, J. A.
Price, S. L.: Anisotropic atom–atom potentials 95

Rasband, P. B., Horsfield, A. P., and Clancy, P.: Tight-binding parameters for silicon–boron interactions with application to boron-defect pairs in crystalline silicon. 71

Ratier, B., *see* Hamer, P. J.
Rickman, J. M., *see* LeSar, R.
Roberts, K. J., *see* Telfer, G. B.
Robertson, I. J., *see* Payne, M. C.
Rosi-Schwartz, B., and Mitchell, G. R.: Extracting and validating force fields for disordered polymeric materials from neutron scattering data 153

Sanchez-Castro, C.: Temperature and field dependence of the thermodynamic and transport properties of $Ce_3Bi_4Pt_3$ 525
Saunders, G. A., *see* Cutroni, M.
Scansen, D., *see* Johanson, R. E.
Senent, M., *see* Bermejo, F. J.
Sevely, J., *see* Moliton, J. P.
Shabat, M. M.: Nonlinear magnetostatic surface waves in a gyromagnetic film . 669
Shimizu, K., *see* Habazaki, H.
Shimizu, K., Kobayashi, K., Thompson, G. E., Skeldon, P., and Wood, G. C.: Anodic oxide films on tantalum: incorporation and mobilities of electrolyte-derived species 461
Silva, P. R. J., *see* Continentino, M. A.
Singh, M., *see* Bhatia, K. L.
Skeldon, P., *see* Habazaki, H.
Skeldon, P., *see* Shimizu, K.
Slater, B., and Drew, M. G. B.: Monte Carlo simulations of the first-order phase transition in vanadium dioxide 59
Sleeckx, E., *see* Tichý, L.
Stipančić, M., *see* Lugomer, S.
Stuart, J. A., and Price, G. D.: Atomistic potentials for $MgSiO_3$ with the orthorhombic perovskite structure 41
Stutzmann, M., *see* Zacharias, M.
Suzuki, M., *see* Bhatia, K. L.

Tao, M., *see* Mohammad, S. N.
Tao, M., Park, D., Mohammad, S. N., Li, D., Botchkerav, A. E., and Morkoç, H.: Electrical conduction in silicon nitrides deposited by plasma enhanced chemical vapour deposition 723
Telfer, G. B., Wilde, P. J., Jackson, R. A., Meenan, P., and Roberts, K. J.: Potential fitting to molecular ionic materials 147
Telley, H., Liebling, T. M., and Mocellin, A.: The Laguerre model of grain growth in two dimensions. I. Cellular structures viewed as dynamical Laguerre tessellations 395
Telley, H., Liebling, T. M., and Mocellin, A.: The Laguerre model of grain growth in two dimensions. II. Examples of coarsening simulations 409
Thompson, G. E., *see* Shimizu, K.
Thompson, G. E., *see* Habazaki, H.
Thomson, D., *see* Payne, M. C.
Thorsteinsson, T., *see* Cooper, D. L.
Tichá, H., *see* Tichý, L.
Tichý, L., Sleeckx, E., Nagels, P., and Tichá, H.: The influence of temperature on the optical absorption edge shift induced by band-gap illumination in thin amorphous $GeSe_2$ films 213
Tolmatchev, A. V., *see* Ivanov-Omskii, V. I.
Trefilov, A. V., *see* Anokhin, A. O.
Trigaud, T., *see* Moliton, J. P.
Tsallis, C., *see* Nobre, F. D.

Udvardi, L.: The effect of charge transfer on the transition temperatures of binary alloys 737

Valarelli, J. V., *see* Continentino, M. A.
Valiev, R. Z., *see* Alexandrov, I. V.
Vignoli, S., Meaudre, R., and Meaudre, M.: Metastable defect creation and annealing under illumination in intrinsic hydrogenated amorphous silicon deposited from helium–silane mixtures 261
Vinckel, J., Hugel, J., and Gasser, J. G.: Electrical resistivity and absolute thermoelectric power of liquid silver–gallium alloys 231

Wang, Z. L., *see* Kang, Z. C.
Wilde, P. J., *see* Telfer, G. B.
Willock, D. J.: Gradient-based fitting of empirical potentials in the presence of a distributed-multipole electrostatic model 127
Wood, G. C., *see* Shimizu, K.
Wood, G. C., *see* Habazaki, H.

Xantheas, S. S.: Significance of higher-order many-body interaction energy terms in water clusters and bulk water 107

Yan, B., Adriaenssens, G. J., and Eliat, A.: Influence of light intensity on hole transport in a-Si:H transient photocurrents 543
Yastrebov, S. G., *see* Ivanov-Omskii, V. I.

Valiev, R. Z., *see* Alexandrov, I. V.

Zacharias, M., Dimova-Malinovska, D., and Stutzmann, M.: Properties of hydrogenated amorphous silicon suboxide alloys with visible room-temperature photoluminescence 799